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Electric field induced energy level shifts in spherical quantum dot

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Abstract: The effects of an electric field on the electronic energy levels in a spherical quantum dot (QD) of wide-gap semiconductors have been theoretically investigated by using the perturbation method and computed for a single GaAs QD. The results have shown that the electric field causes lowering in the electronic energy levels, the lowering being maximum for the ground level. The field induced shifts in energy levels are also found to increase with the increase in the box dimension. The comparison of the field induced shifts in ground levels of a spherical and a cubic QD has proved a spherical QD to be more sensitive to applied field than a quantum cube.

Keywords: Semiconductor quantum dot, Electro-optic effect

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1. Introduction

The modulations of sharp excitonic resonances by external electric field promise versatile devices, which could serve important functions in future information processing systems. Quantum wells (QW) possess very good modulation properties compared to bulk semiconductors[1,2]. Again, the results of a number of studies on electro-optic effects in quantum wires and dots indicate improvements in the modulation properties over their QW counterparts[3,4]. Indeed, as one goes towards systems with lower dimensionality, modulation properties are expected to greatly enhance due to higher degree of carrier confinement[5]. As a result, studies on electro-optic effects in structures like quantum dots (QD) have been the subject of immense recent interest in the field of optoelectronics. In the present communication, the electric field induced shifts of energy levels of electrons confined in a spherical QD of wide-gap semiconductors will be estimated theoretically. The calculated shifts will be computed for GaAs QD, taking GaAs as a typical example of wide-gap semiconductor. The field induced shift in the ground level of a spherical and a cubic quantum dot of same dimension will also be compared.

2. Theoretical background

A semiconducting sphere of radius R ($\sim$ nm) is assumed to have infinite potential at its surface and zero potential within it. An uniform electric field F_e lying in the range of (0-10^6) V/m is applied in the polar direction (i.e. z-direction) of the spherical dot. The perturbation method has been employed to estimate the shifts in the electronic energy levels due to an electric field. In the present analysis, the above range of the applied field has been chosen due to the fact that the perturbation method yields reasonable results for low electric fields. For fields higher than 10^7 V/m, the voltage drop across the dot may be comparable to the barrier height making the assumption of infinite barrier QD no more valid.

In absence of electric field, the wave function of electrons confined within the above spherical QD can be obtained from the solution of Schroedinger equation, expressed in polar co-ordinate, as[6]

$$\psi_{nlm} = Y_{lm}(\theta,\phi)\frac{1}{R}\left(\frac{2}{r}\right)^{1/2}\frac{J_{l+1/2}(k_{nl}r)}{J_{l+3/2}(k_{nl}R)} \tag{1}$$

where, $Y_{lm}(\theta,\phi)$ is the angle dependent part and the balance represents the radial part. Here, $J_{l+1/2}(k_{nl}r)$ and $J_{l+3/2}(k_{nl}R)$ are Bessel functions of order $(l+1/2)$ and $(l+3/2)$ respectively, k_{nl} is the wave number corresponding to energy value E_{nlm}, $l(=0,1,2,3,....)$ is the angular momentum quantum number, and $m(=0, \pm 1, \pm 2,....,\pm l)$ is the magnetic quantum number.
The energy E_{nlm}, of the n-th level is obtained from the n-th root of the equation

$$J_{l+1/2}(kR) \quad 0 \tag{2}$$

Treating the electric field as a perturbation, the Hamiltonian in the presence of the field F can be expressed as

$$H = H_0 + H_{\rm per}$$

where, H_0 is the unperturbed Hamiltonian and $H_{\rm per} = -\,eFz = -\,eFr\cos\theta$ is the perturbation Hamiltonian, θ being the polar angle. The field F appearing in the expression for H_{per} is the field inside the quantum dot related to the external field F_e by the well-known expression $F = F_e\ 3\epsilon_e/(\epsilon_d + 2\epsilon_e)$, where ϵ_d and ϵ_e are the dielectric constants of the QD and the embedding material respectively.

The perturbation method yields the energy levels, corrected to the second order in F, as

$$E = E_{nlm} + \Delta E^{(1)}_{nlm} + \Delta E^{(2)}_{nlm} \tag{4}$$

where $\Delta E^{(1)}_{nlm}$ and $\Delta E^{(2)}_{nlm}$ are the first and the second order correction terms respectively. However, due to orthogonal property of spherical harmonics, the first order correction term vanishes. The second order correction term can be expressed in Dirac's notation as

$$\Delta E^{(2)}_{nlm} = \sum_{n',l',m'} \frac{|< n', l', m'|\, H_{per}\, |n, l, m >|^2}{E_{nlm} - E_{n'l'm'}} \tag{5}$$

substitution of the value of H_{per}, and after some mathematical manipulation, the energy level shift due to electric field F is finally obtained as

$$\Delta E^{(2)}_{nlm} = \sum_{n'} \frac{|I_1|^2}{E_{n,l,m} - E_{n',l+1,m}} + \sum_{n'} \frac{|I_2|^2}{E_{n,l,m} - E_{n',l-1,m}} \tag{6}$$

where

$$I_1 = -\frac{2eF}{R^2} \frac{b_{lm}}{J_{l+3/2}(k_{nl}R) J_{l+5/2}(k_{n',l+1}R)} I'_1 \tag{7}$$

$$I_2 = -\frac{2eF}{R^2} \frac{b_{l-1,m}}{J_{l+1/2}(k_{n',l-1}R) J_{l+3/2}(k_{nl}R)} I'_2 \tag{8}$$

with

$$I'_1 = \int_0^R J_{l+3/2}(k_{n',l+1}r) J_{l+1/2}(k_{nl}r) r^2 dr \tag{9}$$

and

$$I'_2 = \int_0^R J_{l+1/2}(k_{nl}r) J_{l-1/2}(k_{n',l-1}r) r^2 dr \tag{10}$$

and

$$b_{lm} = \left[\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right]^{1/2} \tag{11}$$

The shift in the ground state energy of an infinite QW of width d ($\sim$ nm) and under the influence of an electric field F, applied along the direction of the well, i.e. the z-direction, has been given by Bastard *et. al.*[7] by a second order perturbation calculation as

$$\Delta E_1^{(2)} = -\frac{1}{24\pi^2}\left(\frac{15}{\pi^2} - 1\right)\frac{m^* e^2 F^2 d^4}{\hbar^2} \quad (12)$$

where the above parameters have the same meaning as in [7].

To compare the field induced shifts in the ground energy levels of a spherical and a cubic QD, we use the equation (12) to estimate the energy shift in the case of a quantum cube of edge d (taken to be equal to 2R) and with an electric field F along the z-direction.

3. Results and discussion

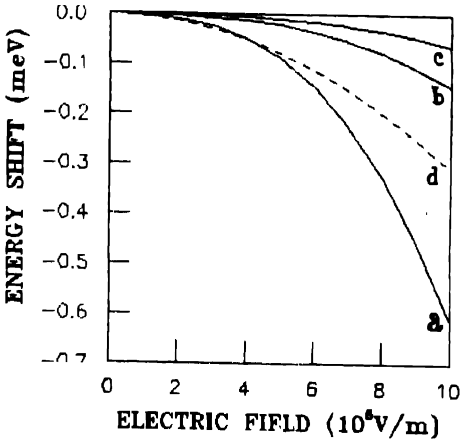

Figure 1. Energy shift vs. applied electric field in the case of ground level of a quantum cube of edge 20 nm (broken, **curve d**), and various levels of a spherical dot of diameter 20 nm (solid) with quantum numbers $l = m = 0$ and $n = 1$ (curve **a**), $n = 2$ (curve **b**) and n=3 (curve **c**).

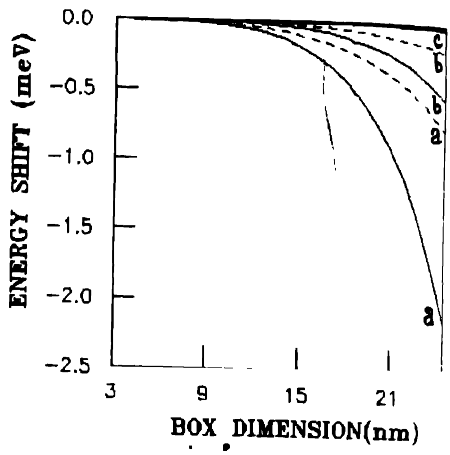

Figure 2. Energy shift vs. box dimension in the case of the ground levels of quantum dots of spherical (solid) and cubic (broken) shape, both having same dimension. Curves are plotted for different electric fields: (**a**) 1 kV/cm, (**b**) 5 kV/cm and (**c**) 10 kV/cm.

The energy shifts in ground and several other low-lying excited levels in spherical QDs have been computed with the material parameters for GaAs[8]. The field induced shifts have been plotted as functions of applied electric field and size of the QD in figures 1 and 2 respectively. In both cases, the ground level shift in a quantum cube of same dimension has also been plotted.

Figure 1 exhibits the shifts in the three energy levels, characterized with the quantum numbers $l=m=0$, $n=1$, 2 and 3 as a function of electric field for a spherical box of dimension 20 nm. For this variation, the energy reference point has been chosen at zero field. The figure shows that as the applied electric field increases, energy levels shift toward low energies. The lowering is found to be most pronounced in the case of the ground level and gradually becomes insignificant for higher lying levels. As evident from the theoretical calculation, the energy lowering is caused by overlapping of wave functions of electrons in various energy levels. In a quantum structure, the interlevel separation decreases towards low energy, resulting maximum overlapping of wave functions. This explains the above observations. Fig.1 also shows that for a particular electric field, the energy shift in the ground level of a cubic QD is relatively small compared to the ground level shift occured in a spherical QD of same dimension. At a field of 10^6 V/m, the ground state energy in a quantum cube of 20 nm edge is lowered by 0.3 meV, whereas the ground state energy lowering in a spherical box with diameter 20 nm is 0.61 meV, i.e., more than double of the earlier one.

The variations of energy shifts in ground levels of a spherical and a cubic QD have been presented in figure 2 as a function of the box dimension for three different values of the electric field. Here, the energy reference point has been chosen at the smallest QD (d=3 nm). In figure 2, the energy lowering is found to be more significant for higher fields, as also observed in figure 1. It is also evident from the figure 2 that for a particular field, shifts in energy levels are much larger for large QDs compared with those for small QDs. In fact, the energy levels of a QD become more crowded with the increase in the box dimension. Therefore, for a large QD, the overlapping of various wave functions become stronger giving rise to a larger energy shift. The figure 2 shows that at a field of 10^6 V/m, the ground state energy in a QD of diameter 20 nm is more than 16 times lowered than that in a QD of diameter 10 nm. Variations of similar nature have been reported by Wen *et. al.*[9] for confined excitons in CdS and $CdS_{0.12}Se_{0.88}$ spherical QDs.

4. Conclusion

In conclusion, the lowering of electronic energy levels of a spherical QD of GaAs due to application of electric field has been shown. The lowering is most pronounced in the case of the lowest energy level. The field induced shift in energy levels increase with the dimension of the spherical dot. A comparison of shift in ground levels has been made for spherical and cubic quantum box. It is seen that the field induced shift is larger for spherical quantum dots. This result is of special significance in the fabrication of practical devices.

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